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Modelling of automotive fuel droplet heating and evaporation: mathematical tools and approximations

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Abstract. New mathematical tools and approximations developed for the analysis of automotive fuel droplet heating and evaporation are summarised. The approach to modelling biodiesel fuel droplets is based on the application of the Discrete Component Model (DCM), while the approach to modelling Diesel fuel droplets is based on the application of the recently developed multi-dimensional quasi-discrete model. In both cases, the models are applied in combination with the Effective Thermal Conductivity/Effective Diffusivity model and the implementation in the numerical code of the analytical solutions to heat transfer and species diffusion equations inside droplets. It is shown that the approximation of biodiesel fuel by a single component leads to under-prediction of droplet evaporation time by up to 13% which can be acceptable as a crude approximation in some applications. The composition of Diesel fuel was simplified and reduced to only 98 components. The approximation of 98 components of Diesel fuel with 15 quasi-components/components leads to under-prediction of droplet evaporation time by about 3% which is acceptable in most engineering applications. At the same time, the approximation of Diesel fuel by a single component and 20 alkane components leads to a decrease in the evaporation time by about 19%, compared with the case of approximation of Diesel fuel with 98 components. The approximation of Diesel fuel with a single alkane quasi-component ($C_{14.763}H_{31.526}$) leads to under-prediction of the evaporation time by about 35% which is not acceptable even for qualitative analysis of the process. In the case when n-dodecane is chosen as the single alkane component, the above-mentioned under-prediction increases to about 44%.

1. Introduction

Modelling of the processes inside internal combustion engines is a challenging task. It includes modelling of coupled fluid dynamics and heat/mass transfer processes in a complex geometry. To take into account the complexity of this geometry, the internal combustion engine chambers should be split up into millions of cells. The parameters of the continuous phase in each of these cells are constant, but they change in time and from one cell to another. Moreover, the dynamics of the dispersed phase (fuel droplets) and chemical reactions in each cell need to be taken into account. The number of these droplets and chemical reactions in each cell can be many thousands in the general case [1, 2].

The above-mentioned features of the modelling of the engine processes make it impossible to perform their rigorous quantitative analysis. Two main approaches have been developed to deal with the complexities of this modelling. The first approach, most widely used in the engineering community, is based on the application of rather simplistic physical models



of individual processes, but the geometry of the enclosure is approximated as accurately as possible. This approach is used in most commercial Computational Fluid Dynamics (CFD) codes. The second approach is focused on in-depth development of the physical models of individual processes, ignoring the complexities of the geometry and details of interactions between various processes. These two approaches do not contradict each other; rather, they are complementary.

In a series of our previous papers, an attempt has been made to develop the third approach to this modelling. This approach is focused on establishing a hierarchy of the processes involved (recognising multiple scales in time and space) and finding a compromise between the accuracy of the models and their CPU efficiency. This allowed us to develop models which were more advanced than those used in the conventional CFD codes, but simple enough to enable their implementation in the above-mentioned codes [3]. Various aspects of this approach were reported at the previous MURPHYS workshops and published in [4]-[8].

In the current paper, the latter approach is illustrated by our modelling of biodiesel and Diesel fuel droplet heating and evaporation, which is an integral part of the spray ignition process in Diesel engines. There will be some overlap with the previously published journal papers [9, 10]. In contrast to these papers, we focus more attention on the mathematical tools and approximations used in our analysis. Also, the models will be illustrated using examples which are different from those given in [9, 10].

2. Basic Equations

The simplest approach to modelling multi-component automotive fuel droplets, widely used in commercial CFD codes, is based on the assumptions that the thermal conductivity of droplets is infinitely large, and the diffusion of species is infinitely fast. The first assumption is commonly justified by the fact that thermal conductivity of droplets is larger than that of ambient air. In the transient processes, typical for internal combustion engines, however, the main parameter describing droplet heating is their diffusivity rather than conductivity. The former is much larger for air than for liquid, which allows us to question the above-mentioned widely used assumption about the droplet's infinitely large thermal conductivity. Regarding the second assumption, it can be questioned based on the estimate of the characteristic time of species diffusivity. This is generally much larger than the characteristic time of thermal diffusivity. Thus, the assumption that multi-component automotive fuel droplets can be approximated by single component droplets (infinitely slow species diffusivity) has more solid physical grounds than the assumption of infinitely fast species diffusivity. In what follows we will show how both these approaches can be relaxed, but in such a way that the model remains simple enough for possible implementation in CFD codes (commercial or research).

The process of heating mono- and multi-component droplets is described by the following transient one dimensional (1D) heat conduction equation for the temperature $T \equiv T(t, R)$ in the liquid phase [11, 12]:

$$\frac{\partial T}{\partial t} = \kappa \left(\frac{\partial^2 T}{\partial R^2} + \frac{2}{R} \frac{\partial T}{\partial R} \right), \quad (1)$$

where $\kappa = k_{\text{eff}}/(c_l \rho_l)$ is the effective thermal diffusivity, k_{eff} , c_l , and ρ_l are the effective thermal conductivity, specific heat capacity, and density respectively, R is the distance from the centre of the droplet (assumed to be spherical), t is time. k_{eff} is linked with the liquid thermal conductivity k_l via the following equation:

$$k_{\text{eff}} = \chi k_l, \quad (2)$$

where the coefficient χ is approximated as [13]:

$$\chi = 1.86 + 0.86 \tanh \left[2.225 \log_{10} \left(\text{Pe}_{d(l)}/30 \right) \right]. \quad (3)$$

This coefficient varies from 1 (at droplet Peclet number $Pe_{d(l)} = Re_{d(l)}Pr_l < 10$) to 2.72 (at $Pe_{d(l)} > 500$). Liquid fuel transport properties and the liquid velocity just below the droplet surface are used for calculating $Re_{d(l)}$.

Equation (1) is solved for $t > 0$ and $0 \leq R < R_d$, where R_d is the droplet radius, with the following boundary condition, assuming that the effects of evaporation can be ignored:

$$h(T_g - T_s) = k_{\text{eff}} \left. \frac{\partial T}{\partial R} \right|_{R=R_d-0}, \quad (4)$$

and the initial condition $T(t = 0) = T_{d0}(R)$, where $T_s = T_s(t)$ is the droplet's surface temperature, $T_g = T_g(t)$ is the ambient gas temperature, h is the convection heat transfer coefficient, linked with the Nusselt number Nu via the following equation $Nu = 2R_d h / k_g$, k_g is the gas thermal conductivity.

To take into account the effect of droplet evaporation, gas temperature is replaced with the effective temperature defined as:

$$T_{\text{eff}} = T_g + \frac{\rho_l L \dot{R}_{de}}{h}, \quad (5)$$

where L is the latent heat of evaporation, \dot{R}_{de} is the rate of decrease of droplet radius due to evaporation (see Equation (13)). R_d is updated at the end of each time step Δt : $R_{d(\text{new})} = R_{d(\text{old})} + \dot{R}_d \Delta t$, where $\dot{R}_d = \dot{R}_{de} + \dot{R}_{ds}$, \dot{R}_{ds} is the change of droplet radius due to swelling (see Equation (13)).

Equations for mass fractions of liquid species $Y_i \equiv Y_i(t, R)$ inside moving but spherically symmetric droplets are presented in the following form [14]:

$$\frac{\partial Y_{li}}{\partial t} = D_{\text{eff}} \left(\frac{\partial^2 Y_{li}}{\partial R^2} + \frac{2}{R} \frac{\partial Y_{li}}{\partial R} \right), \quad (6)$$

where $i = 1, 2, 3, \dots$, D_{eff} is the effective mass diffusivity, linked with the liquid diffusivity D_l via the following equation

$$D_{\text{eff}} = \chi_Y D_l, \quad (7)$$

the coefficient χ_Y varies from 1 to 2.72 and can be approximated as:

$$\chi_Y = 1.86 + 0.86 \tanh \left[2.225 \log_{10} \left(Re_{d(l)} Sc_l / 30 \right) \right], \quad (8)$$

$Sc_l = \nu_l / D_l$ is the liquid Schmidt number, ν_l is the liquid kinematic viscosity. As in the case of k_{eff} , liquid fuel transport properties and the liquid velocity just below the droplet surface were used for calculating $Re_{d(l)}$. The model based on Equations (7) and (8) is known as the Effective Diffusivity (ED) model. The model, based on the assumption that species diffusivity is infinitely fast ($D_{\text{eff}} = \infty$) is referred to as the Infinite Diffusivity (ID) model. The combined ITC/ID model is sometimes known as a well-mixed model. In the opposite limiting case, when there is no species diffusivity ($D_{\text{eff}} = 0$), the multi-component fuel can be dealt with as a mono-component one.

Equation (6) is solved with the following boundary condition [14]:

$$\alpha(\epsilon_i - Y_{lis}) = -D_{\text{eff}} \left. \frac{\partial Y_{li}}{\partial R} \right|_{R=R_d-0}, \quad (9)$$

and the initial condition $Y_i(t = 0) = Y_{i0}(R)$, where $Y_{lis} = Y_{lis}(t)$ are liquid components' mass fractions at the droplet's surface,

$$\alpha = \frac{|\dot{m}_d|}{4\pi \rho_l R_d^2}, \quad (10)$$

\dot{m}_d is the droplet evaporation rate. In the case of mono-component droplets, their evaporation rate is estimated from the following equation [15]:

$$\dot{m}_d = -2\pi R_d D_v \rho_{\text{total}} B_M \text{Sh}, \quad (11)$$

where D_v is the binary diffusion coefficient of vapour in air, B_M is the Spalding mass transfer number defined as:

$$B_M = \frac{\rho_{vs} - \rho_{v\infty}}{\rho_{gs}} = \frac{Y_{vs} - Y_{v\infty}}{1 - Y_{vs}}, \quad (12)$$

Y_{vs} and $Y_{v\infty}$ are the vapour mass fractions near the droplet surface and in the ambient gas, Sh is the Sherwood number (equal to 2 for an isolated stationary droplet).

When calculating the value of \dot{R}_d we took into account both droplet evaporation during the time step, and the change in liquid density during this time step (see Equation (20) in [16]):

$$\dot{R}_d = \dot{R}_{de} + \dot{R}_{ds} = \frac{\dot{m}_d}{4\pi R_d^2 \rho_l} + \frac{R_d(\bar{T}_0)}{\Delta t} \left[\left(\frac{\rho(\bar{T}_0)}{\rho(\bar{T}_1)} \right)^{1/3} - 1 \right], \quad (13)$$

where \bar{T}_0 and \bar{T}_1 are average droplet temperatures at the beginning $t = t_0$ and the end of the time step $t = t_1$, $\Delta t = t_1 - t_0$.

To calculate the species mass evaporation rate \dot{m}_{di} , we calculate first the values of Y_{vsi} . The latter depend on the partial pressure of species i in the vapour state in the immediate vicinity of the droplet surface [17]:

$$p_{vsi} = X_{lsi} \gamma_i p_{vsi}^*, \quad (14)$$

where X_{lsi} is the molar fraction of the i th species in the liquid near the droplet surface, p_{vsi}^* is the partial vapour pressure of the i th species in the case when $X_{lsi} = 1$, γ_i is the activity coefficient. In the limit when $\gamma_i = 1$, Equation (14) describes Raoult's law. This law is assumed to be valid in our analysis.

3. Approximations

The rigorous coupled numerical solutions of the equations described in the previous section would not only require substantial computer power, but would be unnecessary for practical engineering applications. In what follows we discuss the approximations which can substantially simplify the analyses of these equations, almost without sacrificing the accuracy of engineering modelling.

Firstly, we can assume that $h = \text{const}$. This assumption would not be acceptable for the whole period of heating of evaporating droplets, but its application for a short time step cannot be questioned except for at the very last stage of droplet evaporation. This assumption allows us to obtain the analytical solution to Equation (1), subject to the earlier mentioned boundary and initial conditions [18]:

$$T(R, t) = \frac{1}{R} \sum_{n=1}^{\infty} \left\{ q_n \exp \left[-\kappa_R \lambda_n^2 t \right] - \frac{R_d^2 \sin \lambda_n}{\|v_n\|^2 \lambda_n^2} \mu_0(0) \exp \left[-\kappa_R \lambda_n^2 t \right] - \frac{R_d^2 \sin \lambda_n}{\|v_n\|^2 \lambda_n^2} \int_0^t \frac{d\mu_0(\tau)}{d\tau} \exp \left[-\kappa_R \lambda_n^2 (t - \tau) \right] d\tau \right\} \sin \left[\lambda_n \left(\frac{R}{R_d} \right) \right] + T_g(t), \quad (15)$$

where λ_n are solutions to the equation:

$$\lambda \cos \lambda + h_0 \sin \lambda = 0, \quad (16)$$

$$\|v_n\|^2 = \frac{R_d}{2} \left(1 - \frac{\sin 2\lambda_n}{2\lambda_n}\right) = \frac{R_d}{2} \left(1 + \frac{h_0}{h_0^2 + \lambda_n^2}\right),$$

$$q_n = \frac{1}{\|v_n\|^2} \int_0^{R_d} \tilde{T}_0(R) \sin \left[\lambda_n \left(\frac{R}{R_d} \right) \right] dR, \quad \kappa_R = \frac{k_{\text{eff}}}{c_l \rho_l R_d^2}, \quad \mu_0(t) = \frac{hT_g(t)R_d}{k_{\text{eff}}},$$

$h_0 = (hR_d/k_{\text{eff}}) - 1$, $\tilde{T}_0(R) = RT_{d0}(R)$. The solution to Equation (16) gives a set of positive eigenvalues λ_n numbered in ascending order ($n = 1, 2, \dots$). The trivial solution $\lambda = 0$ is not considered.

Solution (15) is valid for $h_0 > -1$, which is satisfied, remembering the physical background of the problem ($h > 0$). In the limit $k_{\text{eff}} \rightarrow \infty$ the prediction of Expression (15) is identical to the one which follows from the model based on the assumption that $k_{\text{eff}} = \infty$ [19] (Infinite Thermal Conductivity (ITC) model).

The value of Nu for an isolated moving droplet is estimated based on the following equation [13]:

$$\text{Nu} = 2 \frac{\ln(1 + B_T)}{B_T} \left(1 + \frac{(1 + \text{Re}_d \text{Pr}_d)^{1/3} \max[1, \text{Re}_d^{0.077}] - 1}{2F(B_T)} \right), \quad (17)$$

where $B_T = \frac{c_{pv}(T_g - T_s)}{L_{\text{eff}}}$ is the Spalding heat transfer number, $F(B_T) = (1 + B_T)^{0.7 \frac{\ln(1+B_T)}{B_T}}$, $L_{\text{eff}} = L + \frac{Q_L}{\dot{m}_d} = \sum_i \epsilon_i L_i + \frac{Q_L}{\sum_i \dot{m}_{di}}$, Q_L is the power spent on droplet heating, c_{pv} is the specific heat capacity of fuel vapour, $\epsilon_i = \epsilon_i(t)$ are the evaporation rates of species i , $\dot{m}_i = \epsilon_i \dot{m}_d$ ($\dot{m}_d = \sum_i \dot{m}_{di}$). The effects of the interaction between droplets are ignored.

Similarly, assuming that $D_{\text{eff}} = \text{const}$ and the same for all species, the system of Equations (6) can be decoupled (this is implicitly assumed in the format of these equations) and each of these equations can be solved analytically as [14]:

$$Y_{li} = \epsilon_i + \frac{1}{R} \left\{ \left[\exp \left[D_{\text{eff}} \left(\frac{\lambda_0}{R_d} \right)^2 t \right] [q_{i0} - Q_0 \epsilon_i] \sinh \left(\lambda_0 \frac{R}{R_d} \right) + \sum_{n=1}^{\infty} \left[\exp \left[-D_{\text{eff}} \left(\frac{\lambda_n}{R_d} \right)^2 t \right] [q_{in} - Q_n \epsilon_i] \sin \left(\lambda_n \frac{R}{R_d} \right) \right] \right\}, \quad (18)$$

where λ_0 and λ_n ($n \geq 1$) are solutions to equations

$$\tanh \lambda_0 = -\frac{\lambda_0}{h_{0Y}} \quad \text{and} \quad \tan \lambda_n = -\frac{\lambda_n}{h_{0Y}} \quad (n \geq 1),$$

respectively, $h_{0Y} = -\left(1 + \frac{\alpha R_d}{D_{\text{eff}}}\right)$.

$$Q_n = \begin{cases} -\frac{1}{\|v_0\|^2} \left(\frac{R_d}{\lambda_0} \right)^2 (1 + h_{0Y}) \sinh \lambda_0 & \text{when } n = 0 \\ \frac{1}{\|v_n\|^2} \left(\frac{R_d}{\lambda_n} \right)^2 (1 + h_{0Y}) \sin \lambda_n & \text{when } n \geq 1 \end{cases} \quad (19)$$

$$q_{in} = \frac{1}{\|v_n\|^2} \int_0^{R_d} R Y_{li0}(R) v_n(R) dR, \quad (20)$$

$n \geq 0$, where

$$v_0(R) = \sinh \left(\lambda_0 \frac{R}{R_d} \right), \quad v_n(R) = \sin \left(\lambda_n \frac{R}{R_d} \right), \quad n \geq 1.$$

The validity of the assumption that D_{eff} is the same for all species can be questioned. However, if this assumption is relaxed then we would need to take into account that D_{eff} becomes

the function of local mass fractions of all species and the system of Equations (6) can no longer be decoupled.

The Sherwood number for isolated droplets Sh can be approximated by the following expression [13]:

$$Sh = 2 \frac{\ln(1 + B_M)}{B_M} \left(1 + \frac{(1 + Re_d Sc_d)^{1/3} \max[1, Re_d^{0.077}] - 1}{2F(B_M)} \right), \quad (21)$$

$Sc_d = \frac{\nu_{air}}{D_v}$ is the Schmidt number, $F(B_M) = (1 + B_M)^{0.7 \frac{\ln(1+B_M)}{B_M}}$. B_T and B_M are linked by the following equation [13]:

$$B_T = (1 + B_M)^\varphi - 1, \quad (22)$$

where

$$\varphi = \left(\frac{c_{pv}}{c_{pa}} \right) \left(\frac{Sh^*}{Nu^*} \right) \frac{1}{Le}, \quad (23)$$

$Le = k_g / (c_{pa} \rho_{total} D_v) = Sc_d / Pr_d$ is the Lewis number,

$$Sh^* = 2 \left(1 + \frac{(1 + Re_d Sc_d)^{1/3} \max[1, Re_d^{0.077}] - 1}{2F(B_M)} \right), \quad (24)$$

$$Nu^* = 2 \left(1 + \frac{(1 + Re_d Pr_d)^{1/3} \max[1, Re_d^{0.077}] - 1}{2F(B_T)} \right). \quad (25)$$

As follows from Equation (23), φ is a function of B_T . Hence, the iteration process needs to be performed to calculate B_T from Equation (22). In our previous paper [20] it was shown that, in some practically important cases, Formula (23) can be simplified assuming that $\frac{Sh^*}{Nu^*} = 1$. This assumption turned out to be too crude in our case.

In the case of multi-component droplets, the problem of modelling droplet evaporation is complicated by the fact that different species diffuse in air at different rates, and the evaporation rate of one of the species is affected by the evaporation rate of other species. Our analysis of \dot{m}_d is based on Equation (11), assuming that the mixture of vapour species can be treated as a separate gas, similar to treating the mixture of nitrogen, oxygen and carbon dioxide as air ($Y_{vs} = \sum_i Y_{vis}$).

The approximations described above lead to the model of multi-component droplet heating and evaporation known as the Discrete Component Model (DCM). In practical engineering applications, this model is applicable to the cases when the number of components is relatively small (about a dozen or so). The most widely used approach to modelling heating and evaporation of droplets with large numbers of components is based on the probabilistic method of analysis (e.g. Continuous Thermodynamics approach [21]-[23] and the Distillation Curve Model [24]). In this approach, a number of additional simplifying assumptions were used, including the assumption that species inside droplets mix infinitely quickly. Models containing features of both approaches are described in [25, 26].

A new approach to modelling the heating and evaporation of multi-component Diesel fuel droplets, suitable for the case when a large number of components is present in the droplets, was suggested in [27]. In this approach it was assumed that the main contribution to automotive fuels (Diesel and gasoline) comes from alkanes, and the contribution of various n-alkanes was described by the distribution function $f_m(n)$ [27]:

$$f_m(n) = C_m(n_0, n_f) \frac{(M(n) - \gamma)^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \exp \left[- \left(\frac{M(n) - \gamma}{\beta} \right) \right], \quad (26)$$

where $n_0 \leq n \leq n_f$, subscripts $_0$ and $_f$ stand for initial and final, $\Gamma(\alpha)$ is the Gamma function, α and β are parameters that determine the shape of the distribution, γ determines the original shift, $M(n) = 14n + 2$ is the molar mass of alkanes,

$$C_m(n_0, n_f) = \left\{ \int_{n_0}^{n_f} \frac{(M(n) - \gamma)^{\alpha-1}}{\beta^\alpha \Gamma(\alpha)} \exp \left[- \left(\frac{M(n) - \gamma}{\beta} \right) \right] dn \right\}^{-1}. \quad (27)$$

This choice of C_m assures that $\int_{n_0}^{n_f} f_m(n) dn = 1$.

Assuming that the properties of hydrocarbons in a certain narrow range of n are close, the continuous distribution $f_m(n)$ was replaced with a discrete one, consisting of N_f quasi-components with carbon numbers

$$\bar{n}_j = \frac{\int_{n_{j-1}}^{n_j} n f_m(n) dn}{\int_{n_{j-1}}^{n_j} f_m(n) dn}, \quad (28)$$

(which are not integers in the general case) and the corresponding molar fractions

$$X_j = \int_{n_{j-1}}^{n_j} f_m(n) dn. \quad (29)$$

where j is an integer in the range $1 \leq j \leq N_f$. Note that $\sum_{j=1}^{N_f} X_j = 1$. The new structures with \bar{n}_j defined by Equation (28) are called quasi-components as they cannot be identified with actual components, characterised by integer n , in the general case, but can be treated as actual components in the analysis of heat and mass transfer processes in complex fuels, using the Discrete Component Model (DCM). The DCM in which the quasi-components are used alongside actual components was called the quasi-discrete model.

It was assumed that all $n_j - n_{j-1}$ are equal, i.e. all quasi-components have the same range of values of n . For the case when $N_f = 1$, this approach reduces the analysis of multi-component droplets to that of mono-component droplets. This model was generalised in [28] to take into account the dependence of density, specific heat capacity, thermal conductivity and viscosity on the values of carbon numbers. It is expected to be particularly useful when N_f is much less than the number of actual species in the hydrocarbon mixture.

There are two main problems with the application of this approach to realistic Diesel fuels. Firstly, even if we restrict our analysis only to alkanes, it does not appear to be easy to approximate their distribution with a reasonably simple distribution function $f_m(n)$, given by Expression (26). Secondly, the contributions of the other hydrocarbon groups, apart from alkanes, cannot be ignored in any realistic model of Diesel fuels. In the model suggested in [10] both of these issues were addressed.

In the new model suggested in [10] the focus is shifted from the analysis of the distribution function to the direct analysis of molar fractions of the components. These are described by the matrix X_{nm} , where n refers to the number of carbon atoms, and m refers to the groups (e.g. alkanes) or individual components (tricycloalkane, diaromatic and phenanthrene). The link between the values of m and the components is shown in Table 1.

m	Component
1	alkanes
2	cycloalkanes
3	bicycloalkanes
4	alkylbenzenes
5	indanes & tetralines
6	naphthalenes
7	tricycloalkane
8	diaromatic
9	phenanthrene

Table 1

For each m the values of \bar{n}_{jm} of quasi-components can be introduced as

$$\left. \begin{aligned} \bar{n}_{1m} &= \frac{\sum_{n=n_{1m}}^{n=n_{(\varphi_m+1)m}} (nX_{nm})}{\sum_{n=n_{1m}}^{n=n_{(\varphi_m+1)m}} X_{nm}}, \\ \bar{n}_{2m} &= \frac{\sum_{n=n_{(\varphi_m+2)m}}^{n=n_{(2\varphi_m+2)m}} (nX_{nm})}{\sum_{n=n_{(\varphi_m+2)m}}^{n=n_{(2\varphi_m+2)m}} X_{nm}}, \\ &\dots\dots\dots \\ \bar{n}_{\ell m} &= \frac{\sum_{n=n_{k_m}}^{n=n_{((\ell-1)\varphi_m+\ell)m}} (nX_{nm})}{\sum_{n=n_{k_m}}^{n=n_{((\ell-1)\varphi_m+\ell)m}} X_{nm}}, \end{aligned} \right\} \quad (30)$$

where $n_{1m}=n_{m(\min)}$ is the minimal value of n for which $X_{nm} \neq 0$, $n_{k_m}=n_{m(\max)}$ is the maximal value of n for which $X_{nm} \neq 0$, $\ell = \text{integer } ((k_m + \varphi_m)/(\varphi_m + 1))$. Parameter φ_m is assumed to be integer; $\varphi_m + 1$ is equal to the number of components to be included into quasi-components, except possibly the last one in the group. φ_m is assumed to be the same for all quasi-components within group m . If $\varphi_m = 0$ then $\ell = k_m$ and the number of quasi-components is equal to the number of actual components. φ_m and k_m depend on m in the general case.

This approach to the generation of quasi-components is based on the selection of the number of components in each quasi-component ($\varphi_m + 1$ in most cases). An alternative approach to their generation can be based on the selection of the number of quasi-components n_{qm} . In this case the number of components in each quasi-component, except possibly the last one, (n_{cm}) is taken equal to the nearest integer of the ratio k_m/n_{qm} . If k_m/n_{qm} is not an integer then the number of components in the last quasi-component (n_{lcm}) is either greater than n_{cm} , if $(k_m/n_{qm}) > n_{cm}$, or less than n_{cm} , if $(k_m/n_{qm}) \leq n_{cm}$. It was found that the second approach is more convenient for practical applications and it was used in [10]. The values of \bar{n}_{im} were calculated using the same approach as in the case presented in Equation (30). Due to the additional dimensions introduced by the subscript m in Equation (30), the new model was called the multi-dimensional quasi-discrete model.

The size of quasi-components controls the number of Solutions (18) to be used in the analysis and ultimately the accuracy of calculations. Another factor affecting this accuracy is the time step used for calculation of droplet heating and evaporation (the ranges of t over which Solutions (18) are used for fixed values of input parameters). This time step is expected to be much shorter than the time steps used for calculation of droplet trajectories. The latter in their turn are much shorter than the time steps used to calculate the parameters of the carrier (gas) phase. Herein lies the multi-rate nature of spray calculations used in computational fluid dynamics (CFD) codes.

4. Results

In this section, the models described in the previous sections are applied to the analysis of heating and evaporation of biodiesel (Discrete Component Model (DCM)) and Diesel (multi-dimensional quasi-discrete model) droplets.

The application of DCM to the analysis of biodiesel fuel droplets can be justified by the presence of the relatively small number of components in these fuels. In [9], the analysis was focused on five types of biodiesel fuels: Palm Methyl Ester (PME) produced from palm oil, Hemp Methyl Esters, produced from hemp seed oil in the Ukraine (HME1) and European Union (HME2), Rapeseed oil Methyl Ester (RME), produced from rapeseed oil in the Ukraine, and Soybean Methyl Ester (SME) produced from soybean oil. These fuels contain up to 15 methyl esters and possibly small amounts of unspecified additives, which were treated as methyl esters with average characteristics. Calculations were performed: (1) taking into account the contribution of all components of biodiesel fuels; and (2) assuming that these fuels can be treated as mono-component fuels with average transport and thermodynamic coefficients.

Following [9] it is assumed that a Butterfat Fatty Acid (BFA) (see Table 5 of [29] for the composition of this fuel) fuel droplet of initial radius $R_{d0} = 12.66 \mu\text{m}$ and initial temperature $T_0 = 300 \text{ K}$ moves with a velocity $U_d = 35 \text{ m/s}$ [30] is considered. As in [9] it is assumed that the gas temperature and pressure are equal to 880 K and 30 bars respectively. The values of droplet surface temperature (T_s) and radius (R_d) versus time (t) for this case are shown in Fig. 1. The calculations were performed: (1) taking into account the contribution of all 9 components of the BFA fuel (multi-component model) and using the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) model; and (2) replacing these components with a single component with average transport and thermodynamic properties obtained as described in Appendix C of [9] (single-component model) and using the Infinite Thermal Conductivity (ITC) model.

As follows from Fig. 1, the droplet temperatures and radii predicted by the multi- and mono-component models are reasonably close. The single component model under-predicts the evaporation time by about 13.4% and droplet surface temperature by up to about 12.0%. These differences are larger than the ones reported in [9] for other types of biodiesel fuel. This implies that biodiesel fuel droplets can be approximated by mono-component droplets with infinitely large thermal conductivities if an accuracy of about 13% can be tolerated.

Following [30], the multi-dimensional quasi-discrete model was tested for the analysis of heating and evaporation of a Diesel fuel droplet of an initial radius $R_{d0} = 10 \mu\text{m}$ and initial temperature $T_0 = 300 \text{ K}$ moving at a velocity $U_d = 35 \text{ m/s}$. As in the case of biodiesel fuel droplets, it is assumed that the gas temperature and pressure are equal to 880 K and 30 bars respectively. The analysis is based on the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) model.

The plots of the droplet surface temperatures T_s and radii R_d versus time for six approximations of Diesel fuel composition are shown in Fig. 2. These are the cases shown in this figure: the contributions of all 98 components are taken into account (indicated as (98)); the contribution of 98 components is approximated by 15 quasi-components/components (indicated as (15)); the contribution of 98 components is approximated by 6 quasi-components (corresponding to the 6 groups mentioned above) and 3 components (tricycloalkane, diaromatic and phenanthrene) without taking into account the diffusion between them so that their mass fractions remain equal to the initial mass fractions and they behave like a single quasi-component (indicated as (S)), the contributions of only 20 alkane components are taken into account (standard approximation used in the original quasi-discrete model [27, 28]) (indicated as (20A)); the contributions of only 20 alkane components are taken into account and these are approximated by a single quasi-component with the average value of the carbon number ($\text{C}_{14.763}\text{H}_{31.526}$, indicated as (SA)), and the approximation of Diesel fuel by n-dodecane. The latter approximation is the one which is most widely used in engineering applications. In the

cases when only the contribution of alkanes was taken into account, the mass fractions of the components were recalculated to ensure that the total mass fractions of all alkanes were equal to 1.

As can be seen from Fig. 2, the values of T_s and R_d predicted by 98 and 15 quasi-component/component approximations are reasonably close. The 15 quasi-component/component approximation under-predicts the evaporation time by about 3.2%. At the same time the single component approximation under-predicts droplet evaporation time by about 19.1% which cannot be accepted in most engineering applications. In the case when Diesel fuel is approximated with 20 alkane components the predicted droplet surface temperatures appeared to be higher and the evaporation time shorter by about 19.2% than in the case of approximation of Diesel fuel with 98 components. This means that the approximation of Diesel fuel with alkanes, a widely used assumption in the modelling of Diesel fuels (see [27, 28] and the references therein), leads to results which are less accurate, compared with the approximation of Diesel fuel by a single quasi-component. The approximation of Diesel fuel with a single alkane quasi-component ($C_{14.763}H_{31.526}$) leads to under-prediction of the evaporation time by about 35.3% which is not acceptable even for qualitative analysis of the process. In the case when Diesel fuel is approximated by n-dodecane, this error increases to about 44.2%. This leads us to question the validity of the results of numerous papers where Diesel fuel was approximated with n-dodecane (see [15, 3] for the details).

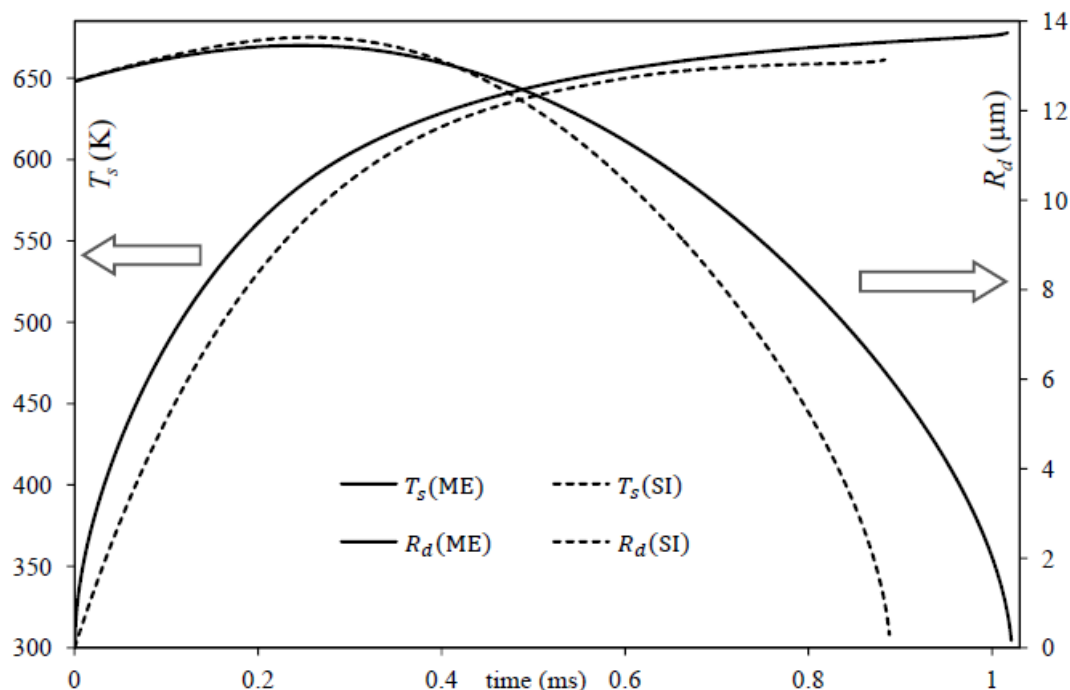


Figure 1. The plots of BFA droplet surface temperatures (T_s) and radii (R_d) versus time predicted by the multi-component (M) and single-component (S) models. Gas temperature and pressure are assumed to be equal to 880 K and 30 bar respectively. The initial droplet radius is assumed to be equal to 12.66 μm and its velocity is assumed to be constant and equal to 35 m/s. The analysis is based on the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) model (E) and Infinite Thermal Conductivity (ITC) model (I).

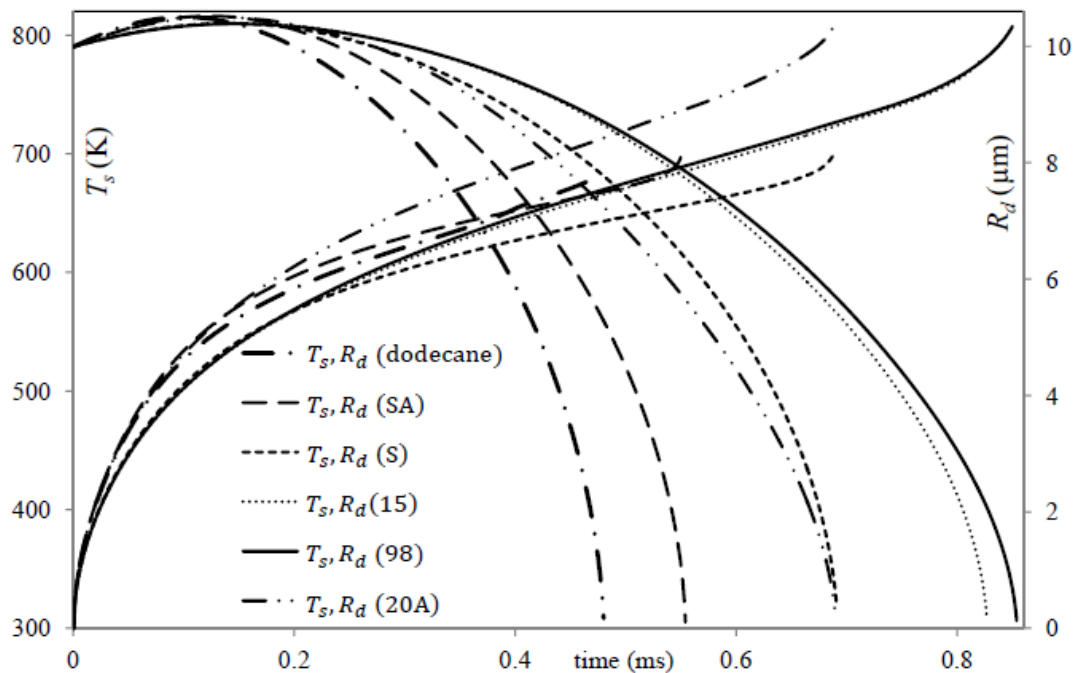


Figure 2. The plots of the droplet surface temperatures T_s and radii R_d versus time for six approximations of Diesel fuel composition, taking into account the contributions of all 98 components (98); 15 quasi-components/components (15); treating Diesel fuel as a single component (S); 20 alkane components (20A); single alkane components (SA) and n-dodecane. Gas temperature and pressure are assumed to be equal to 880 K and 30 bar respectively. The initial droplet radius is assumed to be equal to 10 μm and its velocity is assumed to be constant and equal to 35 m/s. The analysis is based on the Effective Thermal Conductivity/Effective Diffusivity (ETC/ED) model.

5. Conclusions

New mathematical tools and approximations developed for the analysis of automotive fuel droplet heating and evaporation have been summarised. The approach to modelling biodiesel fuel droplets is based on the application of the Discrete Component Model (DCM) in combination with the Effective Thermal Conductivity/Effective Diffusivity model and the implementation in a numerical code of the analytical solutions to heat transfer and species diffusion equations inside droplets. It is shown that the approximation of BFA biodiesel fuel by a single component, using the Infinite Thermal Conductivity model, leads to the under-prediction of droplet evaporation time by about 13% which can be acceptable as a crude approximation in many engineering applications.

The approach to modelling Diesel fuel droplets is based on the application of the recently developed multi-dimensional quasi-discrete model. The application of this model has been combined with the application of the Effective Thermal Conductivity/Effective Diffusivity model and the implementation of the analytical solutions to heat transfer and species diffusion equations inside droplets in the numerical code, as in the case of biodiesel fuel droplets.

The composition of Diesel fuel has been simplified and reduced to only 98 components. It has been pointed out that in contrast to biodiesel fuel droplets, the approximation of Diesel fuel by a single component leads to under-estimation of droplet evaporation time by more than 19%, which is not acceptable in many engineering applications. The approximation of

98 components of Diesel fuel by 15 quasi-components/components leads to under-prediction of this time by about 3% which is believed to be acceptable in most applications. At the same time, the approximation of Diesel fuel with 20 alkane components leads to the prediction of higher droplet surface temperatures and shorter evaporation time than in the case of approximation of Diesel fuel with 98 components. This means that the approximation of Diesel fuel with alkanes, a widely used assumption in the modelling of Diesel fuels, leads to results which are less accurate, compared with the approximation of Diesel fuel by a single quasi-component. The approximations of Diesel fuel with a single alkane quasi-component ($C_{14.763}H_{31.526}$) and n-dodecane lead to under-prediction of the evaporation time by about 35% and 44% respectively, which is not acceptable even for qualitative analysis of the process.

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